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— SECTION A —

PHYSICAL SCIENCES

Contents

SPECIFIC HEATS OF MANGANESE AND BISMUTH AT LIQUID HYDROGEN TEMPERATURES[1]

BY L. D. ARMSTRONG AND H. GRAYSON-SMITH

Abstract

New measurements of the specific heats of manganese and bismuth in the temperature range 14° to 22° K. are reported. The specific heats of these metals are compared with theory. In both cases the approximate theoretical formula

$$C_v = C_D(T/\Theta) + AT,$$

where $C_D(x)$ is the Debye function, is accurately obeyed over the limited temperature region concerned. However, comparison with measurements at other temperatures shows that this may lead to erroneous conclusions. For manganese a precise conclusion is not possible, and it is estimated that the electronic specific heat coefficient A lies between 0.0035 and 0.0040, while Θ varies with temperature from 365 to 390 degrees. For bismuth it is concluded that the electronic specific heat is negligible. This permits an accurate determination of Θ, and it is found that the variation of Θ with temperature is remarkably similar to that predicted by Blackman for a simple cubic lattice.

Introduction

The investigation to be reported here is part of a program of research on the specific heats of metals, and is a continuation of the work of Elson, Grayson-Smith, and Wilhelm (4) on the specific heat of manganese.

According to the approximate theoretical treatment (8, Chaps. I and IV) the specific heat at constant volume of a metal should be given by

$$C_v = C_D(T/\Theta) + AT. \qquad (1)$$

The first term represents the vibrations of the crystal lattice, where $C_D(x)$ is the Debye specific heat function, and Θ is the Debye characteristic temperature. The second term represents the contribution of the conduction electrons, which is linear in T except at very high temperatures. For low temperatures, $T \ll \Theta$, Equation (1) reduces to

$$C_v = 464(T/\Theta)^3 + AT \quad \text{cal. per mole per deg.} \qquad (2)$$

Equations (1) and (2), with constant Θ, are derived on the assumption that the lattice vibrations have a frequency distribution given by the function

$$q(\nu) = b\nu^2, \qquad (3)$$

as for a continuous medium in which the velocity is independent of frequency. Blackman (2, 3) has examined in detail the vibration spectra of some of the common crystal lattices, and has shown that the approximation of Equation

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(3) is unsatisfactory in many cases. This causes deviations from the Debye formula, and it has become customary to take these into account by treating Θ as a function of temperature. For example, Blackman has shown that the curve of $\Theta(T)$ against T may have the form shown in Fig. 1, for a simple cubic lattice with certain assumed values of the interatomic forces.
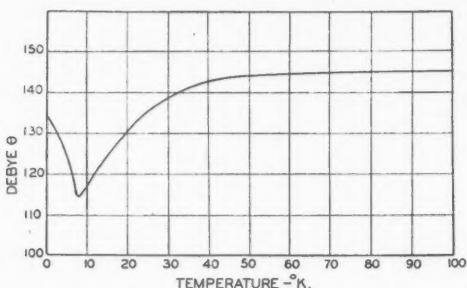
FIG. 1. *The Debye constant Θ as a function of temperature for a simple cubic lattice (after Blackman).*

For comparison with experiment a useful theoretical approximation for the electronic specific heat is (8, p. 181).

$$AT = 3.61 \times 10^{22}(m/\alpha)n^{1/3}V^{2/3}T, \tag{4}$$

where n is the number of conduction electrons per atom, and V is the atomic volume. m/α is the "effective mass", that is, the average inertial mass as determined by the quantum-mechanical relation between the energies and momenta of electron-waves moving through the crystal lattice. A contribution of the form (4) is expected from each unfilled electronic energy band; where the band is nearly filled, n is the number of unoccupied "holes". For a monovalent metal, assuming $\alpha = 1$, A is of order 10^{-4} cal. per mole per deg.[2], but much larger values can be obtained for metals which have overlapping energy bands. This is the case for the transition metals, where large values of the electronic specific heat are attributed to unoccupied holes in the low-lying d-band.

Method

The apparatus and method used were identical with those described by Elson *et al.* (4). The manganese was in the form of a fine powder. It was believed to be of high purity, but an analysis was not available; it may have contained a certain amount of oxide owing to the large proportion of surface exposed. For the measurements, 44.188 gm. of the powder was compressed into the calorimeter. The bismuth was Hilger spectroscopic material, with a purity of 99.998%. It was melted in vacuum to the approximate shape, and machined to fit tightly into the tapered calorimeter chamber. The mass of the sample was 56.258 gm.

The temperatures were determined by the same constantan resistance thermometer as used by Elson. This thermometer has a nearly linear resistance–temperature curve over the range concerned, with an average increase of resistance of about 0.07 ohm per deg. Owing to the excellent thermal contact within the calorimeter, and the small temperature intervals used (about $\frac{1}{2}°$), the cooling curves were nearly straight lines, and the corrected temperature rise could be calculated with ease.

The quantity measured is the specific heat at constant pressure, but the correction to constant volume is negligible at the temperatures concerned, and the measured values may be compared directly with the theoretical formulae.

Manganese

The measurements for manganese are given in Table I, and the experimental values of the specific heat are shown graphically in Fig. 2. Included in the graph are the values given by Elson *et al.* (4), which are about 2% lower than the present measurements. The scattering of the individual values is appreciably less for the present measurements, and it is believed that more time

TABLE I

SPECIFIC HEATS OF MANGANESE

Run No.	Temperature, degrees Kelvin	Time of heating, sec.	Change in temperature, degrees Kelvin	Total heat capacity, Cal./°K.	Calorimeter heat capacity, Cal./°K.	Sample heat capacity, Cal./°K.	Specific heat $C_p = C_v$ Cal./mole/°K.
1	16.24	11.63	0.5180	0.1581	0.0745	0.0836	0.1039
	17.07	12.31	0.4878	0.1747	0.0878	0.0869	0.1080
	17.65	12.58	0.4609	0.1892	0.0973	0.0919	0.1143
	18.08	14.15	0.4932	0.1984	0.1046	0.0938	0.1166
	18.43	16.12	0.5341	0.2092	0.1108	0.0984	0.1224
1	18.62	13.89	0.4522	0.2130	0.1143	0.0987	0.1228
	18.92	14.48	0.4497	0.2232	0.1199	0.1034	0.1287
	19.25	15.28	0.4551	0.2330	0.1263	0.1067	0.1327
	19.53	15.62	0.4492	0.2413	0.1320	0.1093	0.1398
	19.83	16.23	0.4499	0.2507	0.1384	0.1123	0.1359
1	20.14	16.97	0.4538	0.2598	0.1451	0.1147	0.1426
	20.55	15.65	0.4868	0.2750	0.1546	0.1204	0.1497
	20.80	13.97	0.4213	0.2836	0.1670	0.1229	0.1528
	21.14	15.76	0.4541	0.2969	0.1697	0.1272	0.1582
	21.39	16.26	0.4558	0.3052	0.1750	0.1302	0.1619
1	21.32	15.46	0.4385	0.3018	0.1733	0.1270	0.1590
	22.02	16.68	0.4460	0.3205	0.1974	0.1331	0.1655
	22.16	16.20	0.4077	0.3403	0.2024	0.1379	0.1715
	22.48	15.35	0.3717	0.3540	0.2141	0.1399	0.1740
2	15.52	9.15	0.4525	0.1418	0.0636	0.0782	0.0973
	16.34	10.14	0.4530	0.1570	0.0745	0.0825	0.1026
	16.81	10.89	0.4502	0.1697	0.0835	0.0862	0.1072
	17.29	11.72	0.4538	0.1811	0.0914	0.0897	0.1115
	17.64	12.34	0.4563	0.1892	0.0972	0.0920	0.1143

and care in making the measurements, and a more careful interpretation of the cooling curves, have resulted in improved accuracy.

The solid curve in Fig. 2 is plotted from the theoretical formula (2), with $\Theta = 417°$ and $A = 0.00441$, and it can be seen that the experimental
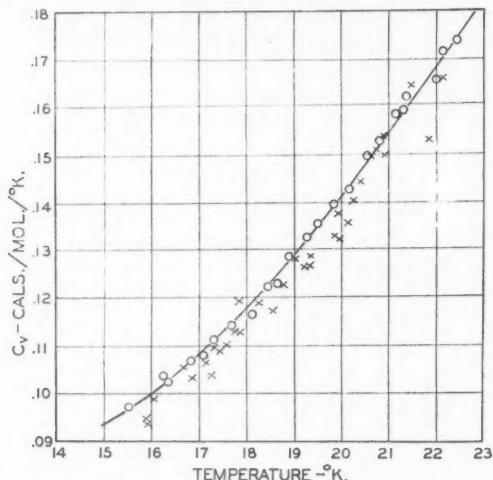
FIG. 2.   *Specific heat of manganese*; ×—*Elson, Grayson-Smith, and Wilhelm*, ○—*Armstrong and Grayson-Smith*.

specific heat is well represented over this limited temperature range by such an equation.   However, these figures have been compared with the measurements made by Kelley (7) in the temperature range 50° to 300° K., and it is evident that the values of Θ and A quoted above are both too large.   It is also evident that there is a sharp variation in $\Theta(T)$ between 15° and 50° K., which makes it impossible to deduce the true value of A accurately.   When Kelley's measurements are corrected to constant volume it is found that $C_v = 6.10$ cal. per gm. per deg. at 290° K.   This implies the existence of a rather large electronic specific heat, and is consistent with a value $A \sim 0.0025$. On the other hand, this very doubtful estimate is clearly too low to agree with the low temperature measurements.   Until measurements in the liquid helium temperature range are available, all that can be done is to assume a value of A, and examine whether $\Theta(T)$, derived from values of $C_v - AT$, has a reasonable temperature dependence.   The conclusion is that A probably lies between 0.0035 and 0.0040.   The derived values of $\Theta(T)$ then vary from 365° to 390°, with a sharp increase through the liquid hydrogen temperature range, and a flat maximum above 22° K.

With this approximate value for the coefficient of the electronic specific heat it is possible to make an estimate of the effective mass coefficient, α, in

Equation (4).   By analogy with the neighboring metals (iron, cobalt, nickel) in the periodic table, manganese should have between 0.5 and 1 free electron per atom in the conducting s-band.   This leaves in the d-band 3.5 to 4 unoccupied holes, which are mainly responsible for the specific heat.   Assuming $n = 3.5$ and $A = 0.0038$ gives m/α approximately equal to 20 electron masses for the electron levels near the top of the occupied region in the d-band.

Bismuth

The measurements for bismuth are given in Table II, and the specific heats are plotted against temperature in a part of Fig. 3.   The curve in this
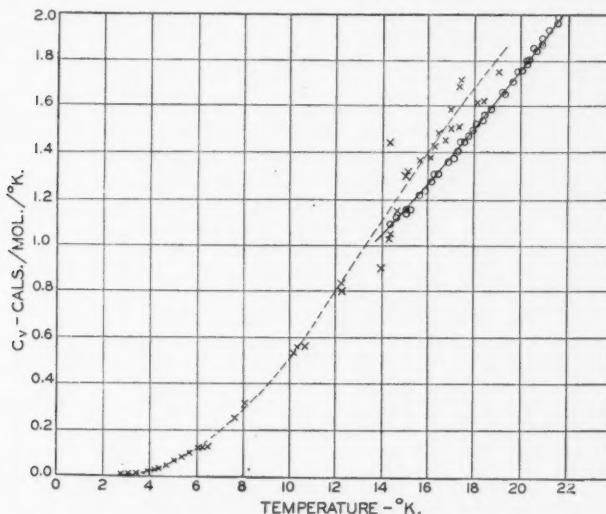
Fig. 3.   *Specific heat of bismuth;* ✕—*Keesom and van den Ende,* ○—*Armstrong and Grayson-Smith.*

figure is empirical, the average deviation of individual values from the smooth curve being 0.6%.   Fig. 3 shows also the measurements made by Keesom and van den Ende (6).   At temperatures where the two sets of measurements overlap, the internal consistency of the present measurements is clearly the better, but the discrepancy still exceeds the probable error of Keesom's measurements.   Keesom did not state either the source or the estimated purity of the material used, and it is possible that the discrepancy is due to impurities.

Over the limited temperature range reported in this paper the measured specific heats agree very accurately with the theoretical formula (1), with $A = 0.060$.   However, when the measurements are compared with those of

TABLE II

Specific heats of bismuth

Run No.	Temperature, degrees Kelvin	Time of heating, sec.	Change in temperature, degrees Kelvin	Total heat capacity, Cal./°K.	Calorimeter heat capacity, Cal./°K.	Sample heat capacity, Cal./°K.	Specific heat $C_p = C_v$ Cal./mole/°K.
1	14.60	15.19	0.3564	0.3558	0.0519	0.3039	1.123
	15.24	15.87	0.3559	0.3719	0.0600	0.3119	1.152
	15.88	17.12	0.3530	0.4042	0.0688	0.3354	1.240
	16.43	18.74	0.3633	0.4300	0.0770	0.3530	1.304
	16.86	17.92	0.3300	0.4524	0.0840	0.3684	1.363
1	17.27	20.87	0.3689	0.4710	0.0907	0.3804	1.406
	20.35	28.32	0.3731	0.6388	0.1494	0.4894	1.809
	20.65	27.87	0.3583	0.6565	0.1563	0.5002	1.850
	20.97	28.41	0.3552	0.6720	0.1644	0.5076	1.876
	21.24	25.10	0.3462	0.6940	0.1716	0.5224	1.931
1	21.60	25.88	0.3482	0.7160	0.1824	0.5336	1.972
	21.91	27.01	0.3501	0.7381	0.1927	0.5454	2.043
	22.23	27.69	0.3487	0.7598	0.2038	0.5560	2.057
2	17.76	20.01	0.3384	0.4997	0.0986	0.4011	1.476
	18.08	21.16	0.3550	0.5174	0.1043	0.4131	1.526
	18.47	21.82	0.3436	0.5364	0.1109	0.4255	1.564
	18.88	24.06	0.3753	0.5508	0.1183	0.4225	1.509
	19.23	23.46	0.3442	0.5748	0.1243	0.4495	1.653
	20.00	25.03	0.3397	0.6204	0.1414	0.4790	1.762
3	15.07	15.75	0.3542	0.3711	0.0577	0.3134	1.158
	15.59	17.31	0.3653	0.3953	0.0643	0.3310	1.223
	16.26	17.29	0.3372	0.4274	0.0744	0.3530	1.304
	17.38	20.04	0.3442	0.4847	0.0924	0.3923	1.450
	20.25	22.73	0.3434	0.6306	0.1470	0.4836	1.789
3	20.59	22.90	0.3288	0.6532	0.1547	0.4985	1.843
	21.21	24.72	0.3382	0.6952	0.1709	0.5243	1.939
	21.64	25.52	0.3360	0.7229	0.1837	0.5392	1.993
	21.96	26.39	0.3376	0.7425	0.1944	0.5481	2.027
	22.25	27.40	0.3402	0.7642	0.2026	0.5616	2.080
4	14.40	13.06	0.3225	0.3415	0.0494	0.2921	1.091
	15.09	15.08	0.3460	0.3678	0.0583	0.3096	1.144
	15.62	16.62	0.3572	0.3922	0.0646	0.3276	1.212
	16.14	17.59	0.3552	0.4180	0.0725	0.3455	1.277
	17.04	18.12	0.3320	0.4597	0.0869	0.3728	1.378
4	17.53	19.84	0.3448	0.4851	0.0948	0.3903	1.443
	17.99	20.36	0.3396	0.5071	0.1025	0.4046	1.495
	18.33	22.93	0.3674	0.5269	0.1085	0.4184	1.547
	18.72	23.43	0.3620	0.5450	0.1155	0.4295	1.589
	19.20	23.60	0.3452	0.5754	0.1247	0.4507	1.667
4	19.62	22.80	0.3642	0.5947	0.1332	0.4615	1.707
	19.93	21.86	0.3386	0.6145	0.1398	0.4747	1.756
	20.26	22.61	0.3392	0.6343	0.1472	0.4871	1.802
	20.58	23.30	0.3382	0.6548	0.1545	0.5003	1.860
	20.91	24.64	0.3467	0.6765	0.1628	0.5137	1.900

Keesom and van den Ende in the liquid helium range, and with those of Anderson (1) at higher temperatures, it is evident that the apparent linear term cannot be attributed to an electronic specific heat. The original measurements of Keesom below 5° K. have been carefully re-examined for any evidence of a linear term, and the conclusion is that the true value of A is less than 5×10^{-5}. This is consistent with estimates of the number of conduction electrons in bismuth. On the basis of measurements of the diamagnetic susceptibilities, Jones (5) estimated 0.0013 electron per atom in the partly filled electronic energy band which is responsible for the conducting properties. Later, Mott and Jones (8, p. 213) gave the still smaller estimate of 10^{-4}. Presumably, the electronic specific heat, if any, would be due to an equal number of unoccupied holes in the nearly filled lower band, but the effective mass would have to be extremely large in order to produce an observable contribution to the specific heat.

It is concluded that the form of the observed specific heat curve of bismuth is entirely due to peculiarities in the spectrum of vibration frequencies in the crystal lattice. Fig. 4 shows the experimental values of $\Theta(T)$, calculated from the smoothed specific heat curve at different temperatures. The similarity of this curve to that calculated by Blackman (Fig. 1) for a simple cubic lattice is remarkable.
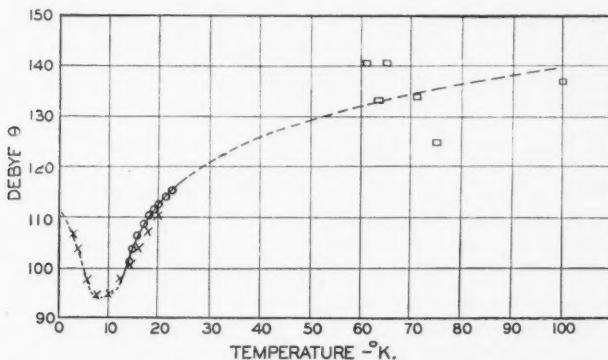

FIG. 4. *Variation of* Θ *with temperature for bismuth;* ×—*Keesom and van den Ende,* □—*Anderson,* ○—*Armstrong and Grayson-Smith.*

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ON THE NUMERICAL CALCULATION OF THE INTERNAL CONVERSION IN THE *K*-SHELL— THE ELECTRIC DIPOLE CASE[1]

By J. P. Stanley

Abstract

Hulme's formula for the internal conversion of γ-radiation is simplified and used to calculate the internal conversion coefficient in the electric dipole case for electrons in the *K*-shell. For each of the elements $Z = 69, 74, 79, 84, 89$, I_K is calculated for 10 values of the variable $\theta = \dfrac{mc^2}{h\nu}$ and a table obtained by interpolation is given for $\theta = 0.05$ to $\theta = 1.70$.

1. Introduction

The theoretical evaluation of the internal conversion of γ-radiation in an atomic system is a well known problem and has been treated by a number of writers. In particular, the case in which the atomic nucleus is assumed to radiate the field of an electric dipole has been treated exhaustively in a paper by H. R. Hulme (1). In his paper, Hulme employs Dirac's relativistic equations and derives formulae for the conversion coefficients I_K and I_{L_I}, corresponding to the electrons of the *K*- and L_I-shells, respectively. Except that screening effects have been neglected, these formulae are exact and enable us to calculate numerical values for I_K and I_{L_I}, if the atomic number Z and the energy of the γ-radiation are assigned.

The quantity which Hulme denotes by I_K and which we use here is such that $2I_K$ corresponds to the ratio of the number of observed *K*-electrons to the number of observed photons of energy $h\nu$. It is perhaps more usual to apply the term 'internal conversion coefficient' to the ratio of the number of observed electrons to the sum of the observed electrons and observed photons (2).

The expressions for I_K and I_{L_I} are extremely complex and the task of calculating numerical values for the various conversion coefficients from such expressions is a formidable one. Although Hulme himself gives the results of calculations for six (6) separate values of I_K corresponding to $Z = 84$ and at least one value for the 'exact' ratio $I_K : I_{L_I}$, in the 16 years since the publication of these results only a very few additional values have been worked out from the 'exact' formulae: however, values of conversion coefficients for other atomic numbers have been estimated from asymptotic formulae and/or by rough interpolation.

Recently, considerable importance has been attached to more exact calculations of conversion coefficients and the present paper contains the results of work done in an attempt to provide a table of I_K values in the electric dipole case.

As a preliminary to the calculations reported here, the formula for I_K, given by Hulme, was simplified. A brief account of the method used and the resulting modified expression for I_K are given in Section 3; Section 2 is devoted to a summary of Hulme's formula. The calculations based on the modified expression for I_K are tabulated in Section 4 and cover the range of atomic numbers from $Z = 69$ to $Z = 89$.

It was originally intended that these calculations should include the tabulation of I_K in the electric dipole case for the complete range of atomic numbers and also tables of conversion coefficients for other electron shells. However, when the work had progressed to the stage reported here, it was learned that one of the large-scale digital computers was being coded to carry out these and more extensive calculations of internal conversion coefficients. Accordingly, the basis of calculation was more or less arbitrary and further work on this problem has been suspended pending a report on progress of the above.

Since some interest may attach to the simplified form of Hulme's expression for I_K which has been obtained, it was decided that these incomplete results should be published. Further, the values of I_K tabulated may be of some value as a rough check on more extensive calculations.

2. Summary of Hulme's Formula for I_K

In the paper referred to earlier, Hulme quotes a final expression for the conversion coefficient I_K which may be written in the form:

$$(2.1) \quad I_K = \frac{1}{24} \frac{\gamma b \theta}{Z} \cdot \frac{(2\gamma)^{2-2\beta}}{\Gamma(3 - 2\beta)(2 - \beta)} \cdot$$

$$\frac{|\Gamma(1 - \beta - ib)|^2}{\left|\left\{\gamma + \frac{i}{\theta}\left(\frac{a}{q} - 1\right)\right\}^{2(1-\beta-ib)}\right|} \times \left\{\frac{2A^2|B|^2}{A^2 + |B|^2}\right\}(2|\mathfrak{A}|^2 + |\mathfrak{B}|^2),$$

where

(2.2)

$$\mathfrak{A} = I_1\left\{\gamma\left(\frac{1}{A} - \frac{2}{|B|}\right) - i\frac{2-\beta}{|B|}\right\} + I_2\left\{\gamma\left(\frac{1}{A} + \frac{2}{|B|}\right) + i\left(\frac{2-\beta}{|B|}\right)\right\}$$
$$+ I_3\left\{\frac{2-\beta}{|B|} + \frac{i\gamma}{A}\right\} + I_4\left\{-\frac{2-\beta}{|B|} + \frac{i\gamma}{A}\right\},$$

and

(2.3)

$$\mathfrak{B} = I_1'\left\{\gamma\left(\frac{1}{A} + \frac{1}{|B|}\right) + i(2 - \beta)\left(\frac{3}{A} - \frac{1}{|B|}\right)\right\}$$
$$+ I_2'\left\{\gamma\left(\frac{1}{A} - \frac{1}{|B|}\right) + i(2 - \beta)\left(\frac{3}{A} + \frac{1}{|B|}\right)\right\}$$
$$+ I_3'\left\{\frac{2-\beta}{|B|} + \frac{i\gamma}{A}\right\} + I_4'\left\{-\frac{2-\beta}{|B|} + \frac{i\gamma}{A}\right\}.$$

The notation used above is essentially the same as that employed by Hulme. For ease of reference this notation is explained below: thus

$$Z = \text{the atomic number.}$$

$$\gamma = \frac{2\pi Z e^2}{ch} = \frac{Z}{137} \quad \text{(approximately)}, \qquad \theta = mc^2/h\nu,$$

where e, m denote the charge and mass of an electron, respectively, and c, h, ν denote, as usual, the velocity of light, Planck's constant, and the frequency of the γ-radiation. It will be noted that θ is a dimensionless parameter corresponding to the energy of the γ-radiation.

$$\beta = 1 - \sqrt{1 - \gamma^2}. \quad \text{(This quantity is the negative of that used by Hulme).}$$

$$q = 2\pi\nu/c.$$

$$A^2 = \frac{2\pi}{h}\left(mc + \frac{E}{c}\right) \qquad\qquad B^2 = \frac{2\pi}{h}\left(mc - \frac{E}{c}\right),$$

where E denotes the final energy of the system considered, i.e., when the electron originally in the K-shell is a free electron outside the atom, and has the value

$$E = mc^2\sqrt{1 - \gamma^2} + h\nu.$$

Three particular expressions involving the quantities A and B are of common occurrence and have been denoted by a, b, and c in Hulme's paper. To avoid possible confusion with the velocity of light, we shall denote these expressions by a, b, and d; they are defined by:

$$AB = ia, \qquad \frac{\gamma}{2}\left(\frac{A}{B} - \frac{B}{A}\right) = -ib, \qquad \frac{\gamma}{2}\left(\frac{A}{B} + \frac{B}{A}\right) = -id.$$

Since, for a free electron, $E \geqslant mc^2$, it follows that B is a pure imaginary and hence that a, b, and d are real.

It remains to define the quantities I_1, I_2, ... I_4': these are complicated expressions involving Gamma functions and hypergeometric functions. In particular

$$I_1 = \bigg\{ F(s + ib + 1, \quad ib - s - 1; \quad ib + \beta; \quad z^{-1})$$

$$(2.4)$$

$$+ \frac{\Gamma(s + 2 - \beta)\ \Gamma(ib + \beta - 1)\ \Gamma(s + 2 - ib)}{\Gamma(s + 1 + \beta)\ \Gamma(s + 1 + ib)\ \Gamma(1 - \beta - ib)} \cdot (-z)^{-(1-\beta-ib)}$$

$$\times F(s + 2 - \beta, \quad -s - \beta; \quad 2 - \beta - ib; \quad z^{-1})\bigg\},$$

$$I_2 = \bigg\{ \frac{s + 1 + ib}{\beta + ib} \cdot z^{-1} \cdot F(s + 2 + ib, \quad ib - s; \quad ib + 1 + \beta; \quad z^{-1})$$

$$(2.4)$$

$$+ \frac{\Gamma(s + 2 - \beta)}{\Gamma(s + 1 + \beta)}\ \frac{\Gamma(ib + \beta)}{\Gamma(s + 1 + ib)}\ \frac{\Gamma(s + 1 - ib)}{\Gamma(1 - \beta - ib)} \cdot (-z)^{-(1-\beta-ib)}$$

$$\times F(s + 2 - \beta, \quad -\beta - s; \quad 1 - \beta - ib; \quad z^{-1})\bigg\} \frac{(k - s) + i(b + d)}{(k - s) - i(b + d)},$$

where

$$s = \sqrt{4 - \gamma^2} - 1,$$

k = an integer which in all cases considered here has the value $+1$,

$$z = \frac{2}{1 - \frac{q}{a} - i\delta},$$

$$\delta = \frac{1}{a \, a_0}, \qquad\qquad a_0 = \frac{h^2}{4\pi^2 m Z e^2},$$

and

arg $(-z)$ is chosen so that $|\text{arg}\,(-z)| < \pi$.

Similar definitions may be given for I_3 and I_4, but these quantities may be calculated from the values of I_1 and I_2, by means of the formulae

$$I_3 = \frac{\frac{a}{q}\left[\delta - i\left(\frac{q}{a} - 1\right)\right]}{(s-\beta+1)(s+\beta+1)V} \cdot \{(\beta - ib) . V\,I_1 + (s - ib + 1)\,(1 - z)I_2\},$$

(2.5)

$$I_4 = \frac{\frac{a}{q}\left[\delta - i\left(\frac{q}{a} - 1\right)\right]}{(s-\beta+1)(s+\beta+1)} \cdot \{(s + ib + 1) . V\,I_1 + (\beta + ib)\,(1 - z)I_2\},$$

where

$$V = \frac{(k - s) + i(b + d)}{(k - s) - i(b + d)}.$$

The remaining quantities I_1' to I_4' are given by formulae analogous to (2.4) and (2.5); we have merely to replace s by s' and $[(k - s) - i(b + d)]$ by $[(b - d) + i(k - 1 - s')]$ in the formulae for I_1 and I_2 and the equations expressing I_3 and I_4 in terms of I_1, I_2. Here, s' is used to denote $[1 - \gamma^2]^{\frac{1}{2}} - 1$, i.e., the negative of β.

3. Modification of Hulme's Formula

Let us begin by defining a new variable ψ, given by

$$\psi = 1 - \beta + 1/\theta.$$

We note that E, the energy of the electron in its final state outside the atom, is given by $mc^2\psi$. Thus ψ is a parameter which measures the ratio of the electron's energy in its final state to the "rest" energy. ψ can have any real value greater than unity: the value unity for ψ is actually critical since it corresponds to a state in which the electron, outside the atom, has no kinetic energy.

In terms of ψ we note the following expressions:

$$A = [q\theta(\psi + 1)]^{\frac{1}{2}},$$

$$|B| = [q\theta(\psi - 1)]^{\frac{1}{2}},$$

$$\frac{2A^2|B|^2}{A^2 + |B|^2} = \frac{q\theta}{\psi}\,(\psi^2 - 1),$$

$$a = q\theta(\psi^2 - 1)^{\frac{1}{2}}$$
$$b = \gamma\psi(\psi^2 - 1)^{-\frac{1}{2}},$$
$$d = \frac{b}{\psi},$$

$$z^{-1} = \frac{1}{2} - \frac{1}{2\sqrt{\psi^2 - 1}}\left(\frac{1}{\theta} + i\gamma\right)$$

$$\frac{1}{\left|\left\{\gamma + \frac{i}{\theta}\left(\frac{a}{q} - 1\right)\right\}^{2(1-\beta-ib)}\right|} = \frac{1}{|(-z)^{-(1-\beta-ib)}|^2}\left[\frac{1}{2(\psi^2 - 1)^{\frac{1}{2}}}\right]^{2-2\beta}e^{b\pi}.$$

Let us now take a factor $\sqrt{q}\theta(\psi^2 - 1)^{\frac{1}{2}}$ into $|\mathfrak{A}|$ and $|\mathfrak{B}|$, combining it with the coefficient of the I's in formulae (2.2) and (2.3). These coefficients now become

(3.1)
$$J_1 = -\gamma(2\mu - \lambda) - i(2 - \beta)\mu,$$
$$J_2 = +\gamma(2\mu + \lambda) + i(2 - \beta)\mu,$$
$$J_3 = +(2 - \beta)\mu + i\gamma\lambda,$$
$$J_4 = -(2 - \beta)\mu + i\gamma\lambda,$$
$$J_1' = +\gamma(\mu + \lambda) + i(2 - \beta)(3\lambda - \mu),$$
$$J_2' = -\gamma(\mu - \lambda) + i(2 - \beta)(3\lambda + \mu),$$
$$J_3' = J_3$$
$$J_4' = J_4,$$

where
$$\lambda = [\theta(\psi - 1)]^{\frac{1}{2}} \quad \text{and} \quad \mu = [\theta(\psi + 1)]^{\frac{1}{2}}.$$

Formulae (2.5), which give I_3 and I_4 in terms of I_1 and I_2, become:

$$I_3 = \frac{i\,\theta\,(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)V}\left[(\beta - ib)z^{-1}\,V\,I_1 + (s + 1 - ib)\,(z^{-1} - 1)I_2\right],$$

(3.2)

$$I_4 = \frac{i\,\theta\,(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)}\left[(s + 1 + ib)z^{-1}\,V\,I_1 + (\beta + ib)\,(z^{-1} - 1)I_2\right].$$

We also define

(3.3)

$$W = \frac{\Gamma(s + 2 - \beta)\,\Gamma(\beta - 1 + ib)\,\Gamma(s + 2 - ib)}{\Gamma(s + 1 + \beta)\,\Gamma(s + 1 + ib)\,\Gamma(1 - \beta - ib)}(-z)^{-(1-\beta-ib)}$$

Combining formulae (2.2), (2.4), and (3.1), we may write, using (3.3),

$$\mathfrak{A}' = \mathfrak{A}_1 + W\,\mathfrak{A}_2,$$

where $\mathfrak{A}' = \theta\,[q\,(\psi^2 - 1)]^{\frac{1}{2}}\,\mathfrak{A}$ and $\mathfrak{A}_1$, $\mathfrak{A}_2$ are complex expressions, which, however, can readily be deduced.

In particular:

(3.4)

$$\mathfrak{A}_2 = J_1 F_2 + V J_2 \left(\frac{\beta - 1 + ib}{s + 1 - ib} \right) F_4$$
$$+ i\theta \frac{(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)} J_3 [(\beta - ib)z^{-1}F_2 + (\beta - 1 + ib)(z^{-1} - 1)F_4]$$
$$+ i\theta \frac{(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)} V J_4 \left[(s + 1 + ib)z^{-1}F_2 + (\beta + ib)(z^{-1} - 1) \right.$$
$$\left. \left(\frac{\beta - 1 + ib}{s + 1 - ib} \right) F_4 \right],$$

where the F_i stand for the following complex hypergeometric functions:

$$F_1 = F(s + 1 + ib, \quad ib - s - 1, \quad ib + \beta, \quad z^{-1}),$$
$$F_2 = F(s + 2 - \beta, \quad - s - \beta, \quad 2 - \beta - ib, \quad z^{-1}),$$
$$F_3 = F(s + 2 + ib, \quad ib - s, \quad ib + \beta + 1, \quad z^{-1}),$$
$$F_4 = F(s + 2 - \beta, \quad - s - \beta, \quad 1 - \beta - ib, \quad z^{-1}).$$

F_1 and F_3 are involved in the corresponding formula for $\mathfrak{A}_1$. If we collect together the coefficients of F_2 and F_4, formula (3.4) may be written in the form

$$\mathfrak{A}_2 = F_2 \left\{ J_1 + \frac{i\theta(\psi^2 - 1)^{\frac{1}{2}}}{z(2 - \beta)} [(\beta - ib)J_3 - (s + 1 + ib) \overline{J_3}V] \right\}$$
$$+ V \frac{(\beta - 1 + ib)}{(s + 1 - ib)} F_4 \left\{ J_2 - i \frac{(z^{-1} - 1)\theta(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)} [(\beta + ib) \right.$$
$$\left. \overline{J_3} - \overline{V}(s + 1 - ib)J_3] \right\}$$

where the bar denotes the complex conjugate.

Let us now introduce

(3.5) $$g = \frac{i\theta(\psi^2 - 1)^{\frac{1}{2}}}{(2 - \beta)} \{(\beta - ib)J_3 + (s + 1 + ib) . VJ_4\} .$$

We then have

(3.6) $$\mathfrak{A}_2 = F_2\{J_1 + z^{-1}g\} + V \frac{(\beta - 1 + ib)}{(s + 1 - ib)} F_4\{J_2 + (z^{-1} - 1)\bar{g}\} .$$

In a similar manner, we obtain the following formula for $\mathfrak{A}_1$,

(3.7) $$\mathfrak{A}_1 = F_1\{J_1 + z^{-1}g\} + z^{-1}V \frac{(s + 1 + ib)}{(\beta + ib)} F_3\{J_2 + (z^{-1} - 1)\bar{g}\}$$

By means of (3.1) we may simplify (3.5); after some algebra, we obtain

$$g = 2\gamma\lambda^2\mu + 2i(1 + \beta)\lambda\mu^2,$$

so that

(3.8) $$J_1 + z^{-1}g = \gamma\mu(\theta - 1) + i[- 3\mu + \lambda(1 + \beta + \theta\{2 - \beta\})]$$

(3.9) $$J_2 + (z^{-1} - 1)\bar{g} = - \gamma\mu(\theta - 1) + i[+ 3\mu + \lambda(1 + \beta + \theta\{2 - \beta\})].$$

Let us denote the quantities given by (3.8) and (3.9) v and w respectively.

Then we have, finally,

(3.91) $|\mathfrak{A}'|^2 = |\mathfrak{A}_1 + W\mathfrak{A}_2|^2$

where

$$\mathfrak{A}_1 = F_1 v + z^{-1}V\frac{(s + 1 + ib)}{(\beta + ib)}\,F_3 w$$

$$\mathfrak{A}_2 = F_2 v + V\frac{(\beta - 1 + ib)}{(s + 1 - ib)}\,F_4 w$$

and W is given by (3.3)

In an exactly parallel manner, we obtain

$$\mathfrak{B}' = \mathfrak{B}_1 + W'\mathfrak{B}_2,$$

where

$$\mathfrak{B}' = \theta[q(\psi^2 - 1)]^{\frac{1}{2}}\mathfrak{B},$$

(3.92) $\mathfrak{B}_1 = G_1\{J_1' + z^{-1}\cdot g'\} + z^{-1}V'\left(\dfrac{1 - \beta + ib}{\beta + ib}\right)G_3\{J_2' + (z^{-1} - 1)\bar{g}'\}$

$$\mathfrak{B}_2 = \{J_1' + z^{-1}\cdot g'\} - V'\{J_2' + (z^{-1} - 1)\bar{g}'\},$$

and

$$g' = i\theta\frac{(\psi^2 - 1)^{\frac{1}{2}}}{\frac{1}{2} - \beta}\{(\beta - ib)J_3 + (1 - \beta + ib)V'J_4\},$$

$$V' = \frac{(b - d) - i(k - 1 + \beta)}{(b - d) + i(k - 1 + \beta)},$$

$$G_1 = F(1 - \beta + ib,\ \ \beta - 1 + ib,\ \ \beta + ib,\ \ z^{-1}),$$

$$G_3 = F(2 - \beta + ib,\ \ \beta + ib,\ \ \beta + 1 + ib,\ \ z^{-1}),$$

W' is obtained by replacing s by $(-\beta)$ in Formula (3.3).

After some algebra, we find

$$g' = \frac{2\gamma}{\beta}\,\lambda\mu(\beta\lambda - i\gamma\mu);$$

whence

$$J_1' + z^{-1}g' = 2(1 - \theta)[\gamma\mu + i\lambda(2 - \beta)]$$

and

$$J_2' + (z^{-1} - 1)\bar{g}' = -2(1 - \theta)[\gamma\mu - i\lambda(2 - \beta)].$$

Substituting in (3.92), we see that

$$\mathfrak{B}_2 = 0$$

Hence

$$|\mathfrak{B}'|^2 = |\mathfrak{B}_1|^2 = 8(2 - \beta)(1 - \theta)^2\left|G_1 + z^{-1}\frac{(1 - \beta + ib)}{(\beta + ib)}G_3\right|^2.$$

But G_1 and G_3 are related by the formula

$$G_1 + z^{-1}\left(\frac{1 - \beta + ib}{\beta + ib}\right)G_3 = (1 - z^{-1})^{-(1 - \beta + ib)}.$$

Therefore

(3.93) $|\mathfrak{B}'|^2 = 8(2 - \beta)(1 - \theta)^2|(1 - z^{-1})^{-(1 - \beta + ib)}|^2.$

Collecting our results, the final formula for the coefficient of internal conversion in the two electrons of the K-shell is

$$(3.94) \quad 2I_K = \frac{\gamma^{3-2\beta}(\psi^2 - 1)^{-(3/2-\beta)}e^{b\pi}|\Gamma(1-\beta-ib)|^2}{12(137)(2-\beta)\Gamma(3-2\beta)|(-z)^{-(1-\beta-ib)}|^2}[2|\mathfrak{A}'|^2 + |\mathfrak{B}'|^2]$$

where

$|\mathfrak{A}'|^2$ and $|\mathfrak{B}'|^2$ are given by (3.91) and (3.93) respectively.

Hulme's formula is far from being stated in its simplest terms and the above modification has simplified the algebra considerably. In particular, we note that the expression for $|\mathfrak{B}'|^2$ no longer involves either Gamma functions or hypergeometric functions. The corresponding simplification holds in the

TABLE I

VALUES OF $2I_K$ (OBSERVED K-ELECTRONS/OBSERVED PHOTONS OF ENERGY $h\nu$)

$\theta = \frac{mc^2}{h\nu}$ Z	89	84	79	74	69
0.05	**0.00007429**	**0.00006297**	**0.00005390**	0.0000439	0.0000354
0.10	**0.0002008**	**0.0001667**	**0.0001393**	0.000113	0.0000914
0.15	**0.0003772**	**0.0003056**	**0.0002530**	0.000206	0.000166
0.20	**0.0005938**	**0.0004769**	**0.0003941**	0.000321	0.000259
0.25	**0.0008497**	**0.0006773**	**0.0005611**	0.000457	0.000368
0.30	0.00115	0.000926	0.000759	0.000616	0.000495
0.35	0.00148	0.00120	0.000983	0.000797	0.000640
0.40	0.00185	0.00151	0.00123	0.00100	0.000805
0.45	0.00226	0.00185	0.00151	0.00123	0.000988
0.50	**0.002706**	**0.002228**	**0.001825**	**0.001485**	**0.001198**
0.55	0.00319	0.00264	0.00217	0.00177	0.00143
0.60	0.00372	0.00309	0.00255	0.00208	0.00169
0.65	0.00430	0.00358	0.00296	0.00242	0.00197
0.70	**0.004922**	**0.004112**	**0.003405**	**0.002797**	**0.002280**
0.75	0.00559	0.00469	0.00389	0.00321	0.00262
0.80	0.00632	0.00532	0.00442	0.00365	0.00299
0.85	0.00709	0.00599	0.00499	0.00413	0.00339
0.90	0.00792	0.00671	0.00560	0.00465	0.00383
0.95	0.00880	0.00749	0.00625	0.00521	0.00430
1.00	**0.009736**	**0.008304**	**0.006956**	**0.005810**	**0.004805**
1.05	0.0107	0.00917	0.00771	0.00645	0.00535
1.10	0.0118	0.0101	0.00851	0.00714	0.00593
1.15	0.0129	0.0111	0.00936	0.00787	0.00655
1.20	0.0141	0.0121	0.0103	0.00865	0.00722
1.25	0.0153	0.0132	0.0112	0.00948	0.00792
1.30	0.0166	0.0143	0.0122	0.0104	0.00867
1.35	0.0180	0.0155	0.0133	0.0113	0.00947
1.40	0.0194	0.0168	0.0144	0.0123	0.0103
1.45	0.0209	0.0182	0.0156	0.0133	0.0112
1.50	**0.02248**	**0.01956**	**0.01687**	**0.01440**	**0.01214**
1.55	0.0241	0.0210	0.0182	0.0156	0.0131
1.60	0.0258	0.0226	0.0196	0.0168	0.0142
1.65	0.0276	0.0242	0.0210	0.0180	0.0153
1.70	**0.02949**	**0.02593**	**0.02253**	**0.01936**	**0.01642**

case of the L_I-shell and will shortly be published. It would seem that the formulae for the other shells can probably be simplified in an exactly parallel manner.

4. The Numerical Calculation of the Coefficients

For each of atomic numbers 89, 84, 79, 74, and 69, formula (3.94) was used to calculate the I_K corresponding to certain selected energy parameters θ. These are shown in bold face in Table I.

The work was carried to five significant digits. It is believed that the fourth digit quoted in the final result is of some value.

The values of the coefficient for intermediate energies were obtained by interpolation, and are quoted to three figures. The interpolation was based on two cubic curves, through the points given by $\theta = 0.25, 0.50, 0.70, 1.00$, and $\theta = 0.70, 1.00, 1.50, 1.70$. It was found that the two arcs agreed very closely in the common range from $\theta = 0.70$, to $\theta = 1.00$, which perhaps lends some justification to the method. Moreover, the calculated values for $\theta = 0.05$ to $\theta = 0.20$ blended fairly well into the interpolation arcs.

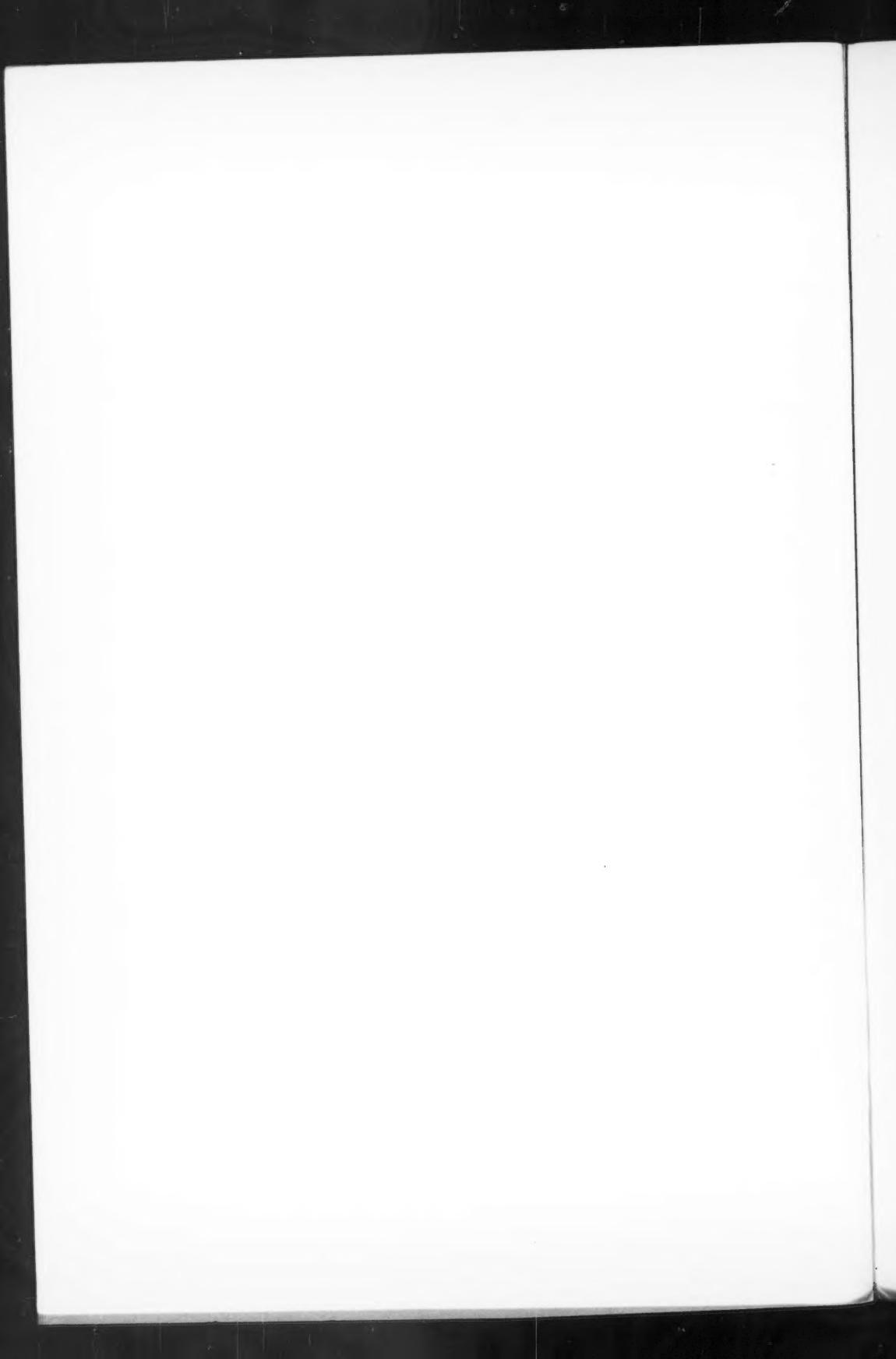The value 1/137 was assumed for the fine structure constant.

Acknowledgment

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